

# LEVEIT



## NAVAL POSTGRADUATE SCHOOL

Monterey, California





### **THESIS**

CLASSIFICATION TECHNIQUES FOR MULTIVARIATE DATA ANALYSIS

by

Jin Ki Lee

March 1980

Thesis Advisor:

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Classification Techniques for Multivariate Data Analysis

by

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Submitted in partial fulfillment of the requirements for the degree of

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#### **ABSTRACT**

The multivariate analysis techniques of cluster analysis, principal components analysis, and discriminant analysis are examined in this thesis. The theory and applications of each of the techniques are discussed. Computer software available at the Naval Postgraduate School is discussed and sample jobs are included.

A hierarchical cluster analysis algorithm, available in the IMSL software package, is applied to a set of data extracted from a group of subjects for the purpose of partitioning a collection of 26 attributes of a weapon system into six clusters of superattributes.

A nonhierarchical clustering procedure, principal components analysis, and discriminant analysis were all applied to a collection of data on tanks considering of twenty-four observations of ten attributes of tanks. The cluster analysis shows that the tanks cluster somewhat naturally by nationality. The principal components analysis and the discriminant analysis show that tank weight is the single most important discriminator among nationality.

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#### I. DISCUSSION OF MULTIVARIATE DATA ANALYSIS

#### A. INTRODUCTION

As a set of statistical techniques, multivariate data analysis is concerned with data collected on several dimensions of the same observations. Techniques can be used for many purpose in the behavioral, mathematical, and administrative sciences - ranging from rigidly controlled experiments to explain relationships assumed to be present in a large mass of data to attempts to cluster similar elements or to find functions of the variables that will best discriminate among preselected subpopulations of the observations.

The heart of any multivariate analysis consists of the data matrix. This matrix is a table that gives the results of a number of observations on a number of variables simultaneously (Table I).

Illustrative Data Matrix

	Variables				
Observations	1	2	3	j ··	· · p
1	x <sub>11</sub>	x <sub>12</sub>	x <sub>13</sub>	× <sub>1j</sub>	x <sub>1p</sub>
2	x <sub>21</sub>	x <sub>22</sub>	<sup>x</sup> 23	x <sub>2j</sub>	x <sub>2p</sub>
•	•	•	•	•	•
•	•	•	•	•	•
•	•	•	•	•	•
i	x <sub>i1</sub>	x <sub>i2</sub>	x <sub>i3</sub>	x <sub>1j</sub>	x <sub>ip</sub>
•	•	•	•	•	•
•	•	•	•	•	•
•	•	•	•	•	•
n	x n1	x n2	x n3	x nj	x np

TABLE I.

The table consists of a set of observations (the n rows) and a set of measurements on those observations (the p columns). Cell entries represent the value  $\mathbf{x}_{ij}$  of observation i on variable j. The values are characteristics of the observations and serve to define the observations in any specific study. The cell values may consist of nominal, ordinal, interval, or ratio-scaled measurements, or various combinations of these across columns.

In a general sense "multivariate" analysis would concern two main features:

- The multivariate character lies in the multiplicity of the p variables, not in the size of the set n.
- 2. The variables are dependent among themselves so that we can not split off one or more from the others and consider it by itself. The variables must be considered together.

There are three characteristics often used as a basis for the classification of multivariate analysis:

- whether one's principal focus is on the objects or on the variables of the data matrix;
- 2. whether the data matrix is partitioned into criterion and independent subsets, and the number of variables in each;
- 3. whether the cell values represent nominal, ordinal, or interval scale measurements.

This classification results in four major subdivisions of interest:

single criterion, multiple predictor
 association, including multiple regression,
 analysis of variance and covariance, and
 two-group discriminant analysis;

- multiple criterion, multiple predictor
   association, including canonical correlation, multivariate analysis of variance
   and covariance, and multiple discriminant
   analysis;
- 3. analysis of variable interdependence, including factor analysis, multidimensional scaling, and other types of dimension-reducing methods;
- analysis of interobject similarity, including cluster analysis and other types of grouping procedures.

The first two categories involve dependence structures where the data matrix is partitioned into criterion and independent subsets; in both cases interest is focused on the variables. The last two categories are concerned with interdependence - either focusing on variables or on observations. Within each of four categories, various techniques are differentiated in terms of the type of scale assumed.

In this research, we consider only the following techniques of multivariate analysis:

- 1. Principal components analysis
- 2. Discriminant analysis
- 3. Cluster analysis

#### II. PRINCIPAL COMPONENTS ANALYSIS

The basic idea of principal components analysis is to describe the dispersion of an array of n points in p-dimensional space by introducing a new set of orthogonal linear coordinates so that the sample variances of the given data points with respect to these derived coordinates are in decreasing order of magnitude. Thus the first principal component is such that the projection of given points onto it have maximum variance among all possible linear coordinates; the second principal component has maximum variance subject to being orthogonal to the first; and so on.

Suppose that the random variables  $\, X_1^{}$  ,  $\, X_2^{}$  , ....,  $\, X_p^{}$  of interest have a certain multivariate distribution with finite mean vector  $\, u \,$  and variance-covariance matrix  $\, \Sigma \,$  .

From this population a sample of n independent observation vectors has been drawn. The observation can be written as the usual nxp data matrix.

$$X = \begin{bmatrix} x_{11} & \dots & x_{ip} \\ \vdots & \vdots & \vdots \\ x_{n1} & \dots & x_{np} \end{bmatrix} = \begin{bmatrix} x'_{1} \\ \vdots \\ x'_{n} \end{bmatrix}$$
 (1)

The estimate of  $\Sigma$  will be the usual sample variance-covariance matrix S defined as follows:

$$S = \frac{1}{n-1} A$$

$$A = \sum_{j=1}^{n} (X_{j} - \bar{X})(X_{j} - \bar{X})'$$
(2)

The information we shall need for our principal components analysis will be contained in S. However, it will be necessary to make a choice of measures of dependence: should we work with the variances and covariances of the observations, and carry out the analysis in original unit of the responses, or would a more accurate picture of the dependence pattern be obtained if each  $x_{ij}$  were transformed to a standarized score

$$z_{ij} = \frac{x_{ij} - \bar{x}_{j}}{s_{i}}$$

and the correlation matrix R employed? The components obtained from S and R in general not the same, nor is it possible to pass from one solution to the other by a simple scaling of the coefficients.

If the responses are in widely different units (i.e., number of crew, weight in tons, speed in kilometer per hour, etc.) with large differences in the magnitudes, linear compounds of original quantities would have little

meaning and standarized variates and correlation matrix should be employed. Conversely, if the responses are reasonably commensurable, the covariance form has a greater statistical appeal, for the i-th principal component is that linear compound of the responses which explains the i-th largest portion of the total response variance, and maximization of such total variance of standard scores is rather artificial.

The first principal component of the complex of sample values of the responses  $\mathbf{X}_1$  ,  $\mathbf{X}_2$  , .....,  $\mathbf{X}_p$  is the linear compound

$$Y_1 = a_{11}X_1 + \dots + a_{p1}X_p$$
 (3)

whose coefficients  $a_{i1}$  are the elements of the eigenvector associated with the greatest eigenvalue  $\lambda_1$  of the sample variance-covariance matrix of the responses. The  $a_{i1}$  are are unique up to multiplication by a scale factor, and if they are scaled so that  $a'_{1}a_{1}=1$ , the eigenvalue  $\lambda_1$  is interpretable as the sample variance of  $Y_1$ .

Numerical representation of the first principal component is to find the vector  $\mathbf{A}_{1}$  such that

$$Y_1 = a_{11}X_1 + \dots + a_{p1}X_p$$

$$= A_1X$$
(4)

which maximizes sample variance

$$s_{Y}^{2} = \sum_{\Sigma}^{p} \sum_{\Sigma}^{p} a_{i1}a_{j1}s_{ij}$$

$$= A'_{1}SA_{1}$$
(5)

for all coefficient vectors normalized so that  $A'_1A_1 = 1$ . To determine the coefficients, the normalization constraint is introduced by means of Lagrange multiplier and the resulting expression is differentiated with respect to  $A'_1$ :

$$\frac{\partial}{\partial A_{1}} [S_{Y_{1}}^{2} - \lambda_{1} (I - A_{1}'A_{1})] = \frac{\partial}{\partial A_{1}} [A_{1}'SA_{1} + \lambda_{1} (I - A_{1}'A_{1})]$$

$$= 2(S - \lambda_{1}I)A_{1}$$
(6)

The coefficients must satisfy the p simultaneous linear equations.

$$(S - \lambda_1 I)A_1 = 0 \tag{7}$$

If the solution to these equation is to be other than the null vector, the value of  $\lambda_1$  must be chosen so that

$$|S - \lambda_1 I| = 0 \tag{8}$$

 $\lambda_1$  is thus an eigenvalue of the variance-covariance matrix, and  $A_1$  is its associated eigenvector. To determine which of the p eigenvalues should be used, premultiply the

the system of equation (7) by  $A_1'$ . Since  $A_1'A_1 = 1$ , it follows that

$$\lambda_1 = A_1' S A_1 = s_{Y_1}^2$$

But the coefficient vecotr was chosen to maximize this variance, and therefore,  $\lambda_1$  must be the greatest eigenvalue of S .

The second principal component is that linear compound

$$Y_2 = a_{12}X_1 + \dots + a_{p2}X_p$$
 (9)

whose coefficients have been chosen, subject to the constraints

$$A_2' A_2 = 1$$
 $A_1' A_2 = 0$ 
(10)

so that the variance of  $Y_2$ ,  $A_2$ 'S  $A_2$ , is a maximum. The first constraint is merely a scaling to assure the uniqueness of the coefficients, while the second requires that  $A_1$  and  $A_2$  be orthogonal.

The coefficients of the second component can also be found by the Lagrangian technique with two multipliers  $~\lambda_2$  and  $~\mu$  . Differentiating this with respect to  $~A_2~$  gives:

$$\frac{\partial}{\partial A_2} [A_2' S A_2 + \lambda_2 (1 - A_2' A_2) + \mu A_1' A_2]$$

$$= 2(S - \lambda_2 I) A_2 + \mu A_1$$
(11)

If the right-hand side is set equal to 0 and premultiplied by  $\mathbf{A_1}'$  , it follows from the normalization and orthogonality conditions that

$$2 A_2' S A_2 + \mu = 0$$
 (12)

Similar premultiplication of the equation (7) by  $A_2$ ' implies that

$$A_2' S A_2 = 0$$
 (13)

and hence  $\mu = 0$ . The second vector must satisfy

$$(S - \lambda_2 I)A_2 = 0 \tag{14}$$

And it follows that the coefficients of the second component are thus the elements of the eigenvector corresponding to the second greatest eigenvalue. The remaining principal components are found in their turn in the same manner from the other eigenvectors.

Thus the j-th principal component of the sample of p-variate observations is the linear compound

$$Y_j = a_{1j}X_1 + \dots + a_{pj}X_p$$
 (15)

whose coefficients are the elements of the eigenvector of the sample variance-covariance matrix S corresponding to the j-th largest eigenvalue  $\lambda_j$ . If  $\lambda_i \neq \lambda_j$ , the coefficients of the i-th and j-th components are necessarily orthogonal; if  $\lambda_i = \lambda_j$ , the elements can be chosen to be orthogonal, although an infinity of such orthogonal vectors exists. The sample variance of the j-th components is  $\lambda_j$ , and the total system variance is thus

$$\lambda_1 + \lambda_2 + \dots + \lambda_p = \text{tr S}$$
 (16)

The importance of the j-th component in a more parsimonious description of the system is measured by

$$\frac{\lambda_{j}}{\text{tr. S}} \tag{17}$$

which gives the fraction of the total variance contributed to the j-th component.

#### III. DISCRIMINANT ANALYSIS

#### A. INTRODUCTION

The basic idea of discriminant analysis consists of assigning an individual from a group of individuals to one of several known or unknown distinct propulations, on the basis of observations on several characters of the individual or group and a sample of observations on these characters from the populations if these are unknown.

Fisher (1936) was the first to suggest a linear function of variables representing different characters, hereafter called the linear discriminant function (discriminator) for classifying an individual into one of two populations. Later research extended the analysis to classification into one of k populations.

For the univariate case Fisher suggested a rule which classifies an observation  $\mathbf{x}$  into the i-th univariate population if

$$X - \bar{X}_{i} = min (X - \bar{X}_{1}, X - \bar{X}_{2}), i = 1,2$$
 (18)

where  $\bar{X}_i$  is the sample mean based on a sample of size  $N_1$  from i-th population. For two p-variate populations  $\pi_1$  and  $\pi_2$  (with the same covariance matrix) Fisher replaced the vector random variable by an optimum linear combination of its components obtained by maximizing the

ratio of the difference of the expected values of a linear combination under  $\pi_1$  and  $\pi_2$  to its standard deviation. He then used his univariate discrimination method with this optimum linear combination of components as the random variable.

Rao (1948) considered the problem of classifying people into one of these populations castes of India. He assumed that each of the three populations could be characterized by four variables - structure  $(x_1)$ , sitting height  $(x_2)$ , nasal depth  $(x_3)$ , and nasal height  $(x_4)$  - of each member of the population. On the basis of sample observations on these characters from the three populations the problem is to classify an individual with observation  $X = (x_1, x_2, x_3, x_4)^T$  into one of three populations. He used a linear discriminator to obtain the solution.

#### B. THEORY

In general, the underlying assumptions of discriminant analysis are:

- 1. the groups being investigated are discrete and identifiable:
- 2. each observation in each group can be described by a set of measurements on p characteristics or variables:
- 3. these p variables are assumed to have a multivariate normal distribution in each population.

The purposes of discriminant analysis are:

- to test for mean group differences and to describe the overlaps among groups;
- 2. to construct classification schemes based upon the set of p variables in order to assign previously unclassified observations to the appropriate groups.

Hence, the problem of studying the direction of group differences is, equivalently, a problem of finding a linear combination of the original independent variables that shows large differences in group means. In short, discriminant analysis is a method for determining scuh linear combinations.

The first step toward determining a linear combination of a set of variables such that several group means on this linear combination will differ widely among themselves, is to decide on a criterion for measuring such group-mean differences. Once a linear combination has been constructed, that means there is just a single transformed variable. Hence, the F-ratio for testing the significance of the over all difference among several group means on a single variable suggests an appropriate criterion.

$$F = \frac{v'Bv}{v'Wv} = \lambda \tag{19}$$

where  $v' = (v_1, v_2, \dots, v_p)$ , a set of weight which maximizes  $\lambda$ .

$$B = \sum_{i=1}^{G} N_{i}(\bar{x}_{i} - \bar{x}_{..})(\bar{x}_{i} - \bar{x}_{..})'$$

$$W = \sum_{i=1}^{G} \sum_{I=1}^{n_i} (x_{ij} - \bar{x}_{i.})(x_{ij} - \bar{x}_{i.})'$$

 $\mathbf{x}_{\mbox{ij}}$  is the jth observation vector in the i-th group.

 $\tilde{\mathbf{x}}$  is the grand mean vector of the data.

G is the number of groups.

 $\mathbf{n}_{\mathbf{i}}$  is the number of observations in the ith group. Prime notation indicates transpose.

This ratio  $\lambda$ , called the discriminant criterion, was originally proposed by Fisher in connection with his two-group discriminant function. Once a criterion for group differentiation has been determined, a set of weights,  $(v_1 \ v_2 \ , \ \ldots, \ v_p)$ , which maximizes this criterion, should be determined. This is accomplished by taking the partial derivative of  $\lambda$  with respect to each component  $v_i$  of v and setting the result equal to zero.

$$\frac{\partial \lambda}{\partial v} = \frac{2[(Bv)(v'Wv) - (v'Wv)(Wv)]}{(v'Wv)^2}$$

$$= \frac{2(Bv - Wv)}{v'Wv} = 0$$
(20)

which is equivalent to

$$(B - \lambda W)v = 0$$

$$(W^{-1}B - \lambda I)v = 0$$
(21)

This equation is of the form

$$(A - \lambda I)v = 0 (22)$$

It's solution, yielding the eigenvalues  $\lambda_p$  and associated eigenvectors  $V_p$  of the matrix A , is therefore the same as in the principal components analysis, and thus the solved problem satisfies the problem of maximizing the discriminant criterion.

In the last equation, the number of non-zero eigenvalues of a square matrix A is equal to the rank of A. With  $W^{-1}B$  playing the role of A, the number of non-zero eigenvalues depends on the rank of B, since the rank of the product of two matrices can not exceed the smaller of the two factor matrices' ranks, and  $W^{-1}$  (being nonsingular) must be of full rank p, while the rank of B is usually smaller than p. Thus it is possible to denote the rank of B by  $r = \min (G-1,p)$ .

From the fact that the eigenvalues  $\lambda_p$  are the values assumed by the discriminant criterion for linear combination using the elements of the corresponding eigenvectors P as combining weights, it is clear that the eigenvector

 $V_1' = (v_{11}, v_{12}, \dots, v_{1p})$  provides a set of weights such that the transformed variable

$$Y_1 = v_{11}X_1 + v_{12}X_2 + \dots + v_{1p}X_p$$
 (23)

has the largest discriminant-criterion,  $\lambda$  , achievable by any linear combination of the p independent variables.

What are the properties of the remaining eigenvectors,  $v_2, v_3, \ldots, v_p$ ? The second discriminant function  $Y_2 = v_{21}X_1 + v_{22}X_2 + \ldots + v_{2p}X_p$  whose weights are the elements of the eigenvector  $v_2$  associated with the second largest eigenvalue  $\lambda_2$  of  $W^{-1}B$  has the largest discriminant-criterion among those linear combinations of the  $X_1$  that are uncorrelated with the first discriminant function in the total sample observation. Its proof is analogous of that of principal components analysis. Each discriminant function has a relative (or conditional) maximum value for its discriminant criterion. Therefore, it needs nonly to show that  $Y_2$  is uncorrelated with  $Y_1$ . Noting that this correlation is proportional to  $v_1'Tv_2$  (where T = W + B), we have to prove that  $v_1'Tv_2 = 0$ .

$$(B - \lambda_i W)v_i = 0$$
 for each i (24)

hence,

 $Bv_1 = \lambda_i Wv_1$  and  $Bv_2 = \lambda_2 Wv_2$ 

premultiplying these equations by  $\mathbf{v}_2$ ' and  $\mathbf{v}_1$ ' respectively,

$$v_2'Bv_1 = \lambda_1 v_2'Wv_1$$
  
 $v_1'Bv_2 = \lambda_2 v_1'Wv_2$ 
(25)

taking the transpose of both sides of the first equation (B and W are symmetric)

$$v_1'BV_2 = \lambda_1 v_1'WV_2$$

thus

$$\lambda_1 V_1 WV_2 = \lambda_2 V_1 WV_2$$

$$(\lambda_1 - \lambda_s) V_1' W V_2 = 0$$

since

$$\lambda_1 \neq \lambda_2$$
,  $V_1$ 'W $V_2 = 0$ 

therefore,  $V_1'WV_2 = 0$  which means  $V_1$  and  $V_2$  are uncorrelated, and  $Y_2$  has this property: its discriminant-criterion value,  $\lambda_2$ , is the largest achievable by any linear combination of X's that is uncorrelated (in the total sample) with  $Y_1$ . Similarly

$$Y_3 = v_{31}X_1 + v_{32}X_2 + \dots + v_{3p}X_p$$
 (36)

has the largest possible discriminant-criterion value  $(\lambda_3)$  among all linear combinations of the X's that are uncorrelated with both  $Y_1$  and  $Y_2$ ; and so on until  $Y_r$  using the

elements of  $V_r$  as weights, has the largest possible discriminant-criterion value among linear combinations that are uncorrelated with all the preceding linear combinations  $Y_1, Y_2, \ldots, Y_{r-1}$ . The linear combinations  $Y_1, Y_2, \ldots, Y_r$  are called the first, second, ...., r th (linear) discriminant functions for optimally differentiating among the g given groups.

The situation here is reminiscent of principal components analysis. There, the dimension corresponding to the first component had maximum variance; the second-component dimension had maximum variance among those uncorrelated with the first; and so on. In discriminant analysis, the ratio of between-to within-groups sums-of-squares merely takes the place of variance as the criterion in determining the successive dimensions. However, an important difference between the dimensions identified in discriminant analysis and those in component analysis is that the former are generally not mutually orthogonal in the test space, even though they are uncorrelated. That is, the axis representing the discriminant functions are not a subset of axes obtainable by rigid rotation of the original system of p axes; the discriminant rotation in an oblique rotation.

Just as in the principal components analysis, the dimensions represented by the discriminant functions may be interpreted meaningfully. Even if they are not, it may be possible to achieve parsimony by reducing the dimensionality of the space needed to describe group differences. In

seeking to interpret the discriminant functions, the goal is to determine which of the original p variables contribute most to each function. For this prupose, comparison of the realtive magnitudes of the combining weights as given by the elements of each eigenvector of W<sup>-1</sup>B is inappropriate because these are weights to be applied to the variables in raw-score scales, and are hence affected by the particular unit used for each variable.

To eleminate the spurious effects of units of measurement on the magnitudes of combining weights, standarized variables should be used.

The relative magnitudes of these standarized weights may be assessed by multiplying each raw-score weight by the standard deviation of the corresponding variable as computed from the within-groups SSCP (Sum of Squares, Cross product) matrix. This amounts to multiplying each element of a given eigenvector  $\mathbf{V}_{\mathbf{m}}$  by the square root of the corresponding diagonal element of W . Thus, for each  $\mathbf{m}$ , define

$$v_{mi}^* - w_{ii} v_{mi}$$
  $i = 1, 2, ..., p$  (27)

as the standarized discriminant weights. The relative contribution of the ith variable to the m th discriminant function may then be gauged by the magnitude of  $v_{mi}^{\;\star}$  in comparison with the other weights  $v_{mj}^{\;\star}$ .

Up to this point, it has been shown that the dimensionality of the discriminant space is equal to the number of

nonzero eigenvalues of  $W^{-1}B$ , which is the smaller of the two numbers,  $G^{-1}$  and p. It may often happen, that the number of significant discriminant dimensions may be even smaller. That is, not all of the discriminant function may represent dimensions along which statistically significant group differences occur.

#### C. SIGNIFICANCE TEST IN DISCRIMINANT ANALYSIS

A basic quantity in testing the significance of the overall difference among several group centroids (mean vectors) the ratio of the determinants of the withingroups and the total SSCP matrices, known as Wilks'  $\Lambda$  criterion.

$$\Lambda = \frac{|W|}{|T|} \tag{28}$$

Motivation for use of this equation may be seen as follows:

$$\frac{1}{\Lambda} = \left| \frac{T}{W} \right| |W^{-1}T| 
= |W^{-1}(W + B)| 
= (1 + \lambda)(1 + \lambda_2); ..., (1 + \lambda_r)$$
(29)

where  $\lambda_1, \lambda_2, \ldots, \lambda_r$  are the nonzero eigenvalues of W<sup>-1</sup>B. Consequently, Bartlet's V statistic for testing the significance of an observed value can be expressed as

$$V = - [N - 1 - (p + G)/2] \ln \Lambda$$

$$= [N - 1 - (p + G)/2] \ln [(! + \lambda_1)(1 + \lambda_r)]$$

$$= [N - 1 - (p + G)/2] \sum_{m = 1}^{\infty} \ln(1 + \lambda_m)$$

$$= [N - 1 - (p + G)/2] \sum_{m = 1}^{\infty} \ln(1 + \lambda_m)$$

This statistic is distributed approximately chi-square with p(G-1) degrees of freedom.

Because of the uncorrelatedness of the successive discriminant functions, the successive terms  $\ln(1+\lambda_m)$  in the last expression above are statistically independent (assuming multivariate normality of the original p variables). As a result, the additive components of V are each approximately distributed as a chi-square variate. More specifically, the m th component,

$$V_m = [N - 1 - (p + G)/2] \ln (1 + \lambda_m)$$
 (31)

is approximately chi-square with p + G - 2m degrees of freedom. It may be readily verified that the sum of the number of degree of freedom (n.d.f) of the r components, that is,  $(p + G - 2) + (p + G = 4) + \dots + (p + G - 2r)$ , is equal to p(G - 1) regardless of whether r = G - 1 or p.

Consequently, when we cumulatively subtract  $V_1, V_2$ , and so on from V, the remainder each time is also a chi-square variate; and these successive remainders become appropriate statistics for testing whether the residual discrimination after removing the first discriminant

function, the first and second discriminant function, and so forth, is statistically significant. The successive test statistics and their n.d.f.'s may be summarized as follows:

Residual After Removing	Approximate - Statistic	n.d.f.
First discriminant Function	v - v <sub>1</sub>	p(G-1) - (p+G-2) = $(p-1)(G-2)$
First 2 discriminant Function	v - v <sub>1</sub> - v <sub>2</sub>	(p-1)(G-2)-(p+G-4) = $(p-2)(G-3)$
First 3 discriminant Function	v - v <sub>1</sub> - v <sub>2</sub> - v <sub>3</sub>	(p-2)(G-3)-(p+G-6) = $(p-3)(G-4)$
	!	
First s discriminant Function	V-V <sub>1</sub> -V <sub>2</sub> -V <sub>3</sub> V <sub>s</sub>	(p-s)(G-(s+1))

As soon as the residual, after removing the first s discriminant functions becomes smaller than the prescribed percentile point (that is, the  $100(1-\alpha)$ th percentile) of the appropriate chi-square distribution, we may conclude that only the first s discriminant functions are significant at that  $\alpha$  level. If the number of significant discriminant functions thus found is smaller than r (as will often be the case), we will have effected a further reduction in the dimensionality of the space required to describe the differences among the G groups from which

our sample groups were drawn. The remaining r-s dimensions may be regarded as immaterial for population differentiation, since our sample differences along these dimensions can be attributed to sampling error.

management the

#### IV. CLUSTER ANALYSIS

#### A. ORIGIN AND THEORY

Clustering is the grouping of similar objects. The principal functions of clustering are to name, to display, to summarize, to predict, and to aid in interpretation of data with many dimensions. Clustering techniques were first developed in the field of biological taxonomy. It is one of several methodologies included in the broader category called classification.

The cluster analysis problem is the last step we consider in the progression of category sorting problems. While in discriminant analysis some part of the structure is known and missing information is estimated from labeled samples, the operational objectives of clustering is to classify new observations, that is, recognize them as members of one category or another. In cluster analysis little or nothing is known about the category structure. All that is available is a collection of observations whose category membership are known. We seek to discover a category structure which fits the observations. The problem may be stated as one of finding the "natural groups", which means to sort the observations into groups such that the degree of "natural association" is high among members of the same group and low between members of different groups.

Cluster analysis techniques have been applied in many fields of study. The literature is both voluminous and diverse, the terminology differing from one field to another. "Numerical taxonomy" is frequently substituted for cluster analysis among biologists, botanists, and ecologists, while some social scientists may refer "typology". Other frequently encountered terms are pattern recognition and partitioning. While discriminant analysis has been studied by statisticians for nearly 45 years, cluster analysis has only recently come to statistical notice. Any method which partition a set of objects into subsets on the basis of measurements taken on every object qualifies as a clustering method.

Most of the well known clustering techniques fall into one of two main categories: (1) hierachical and (2) non-hierachical (partitioning). The former is one in which every cluster obtained at any stage is a merger of clusters at previous stages. The nonhierachial procedures however form new clusters by lumping and splitting old ones. We consider both categories shortly.

In a geometric sense, every observation may be viewed as a point in p-dimensional Euclidean space. This swarm of data points may contain dense regions or "clouds" of data points which are separable from other regions containing a low density of points. These denser regions constitute what are known as clusters. In one and two dimensional cases, it is easy to visualize and to detect the clusters from scatter

Manager our selection.

plots, assuming that the clusters exist. In higher dimensions, clustering becomes extremely difficult without the aid of a computer.

Mathematical clustering techniques usually require a measure of similarity to be defined for every pairwise combination of the entities to be clustered. In order to solve the cluster problem, it is desirable to define the terms "similarity" and "difference" in a quantitative fashion. A researcher would assign two observations to the same group if the distance between them is sufficiently small, or to different clusters if this distance is sufficiently large.

At this point, two questions may be brought on. The first one is "how do we measure the distance between the observations?" and the second one is "how small is small enough?" and how large is large enough? These will be discussed in the following sections.

#### B. MEASURES OF DISTANCE

#### 1. General

Let  $E_p$  be a symbolic representation for a measurement in p-dimensional space and let X,Y, and Z be any of these points in  $E_p$ . Then any nonnegative realvalued function D(X,Y) satisfying the following conditions qualifies as a distance function (or metric).

- 1. D(X,Y) = 0 if and only if X = Y
- 2.  $D(X,Y) \ge 0$  for all X and Y in  $E_D$

- 3. D(X,Y) = D(Y,X)
- 4.  $D(X,Y) \leq D(X,Z) + D(Y,Z)$

Many clustering algorithm assume such distances given and set about constructing clusters of objects within which the distances are small. The choice of distance function is no less important than the choice of variables to be used in the study. A serious difficulty in choosing a distance lies in the fact that a clustering structure is more primitive than a distance function and that knowledge of clusters changes the choice of distance function. Thus a variable that distinguishes well between two established clusters should be given more weight in computing distances than a "junk" variable that distinguishes badly.

# 2. Euclidean Distance

The Euclidean distance between the I-th and K-th observations of a data matrix X is defined as

$$D(I,K) = \begin{bmatrix} \Sigma & \{X(I,J) - X(K,J)\}^2 \end{bmatrix}^{1/2}$$
(32)

where J is J-th variable. In one, two, or three dimensional space, this is just a "straight line" distance between the vectors corresponding to the I-th and K-th observations. When the variables are measured in different units, it is necessary to prescale the variabes to make their values comparable or, equivalently, to compute a weighted Euclidean distance.

$$D(I,K) = \left[ \sum_{1 \le J \le p} W(J) (X(I,J) - (X(K,J))^{2} \right]^{1/2}$$
 (33)

This form of distance is not necessary if all variables are measured on the same scale. However, even in this case, weights might be used to increase or decrease the importance of same variable. Various weighting schemes have been utilized in practice. One common weighting scheme lets W(J) be the reciprocal of the variance of variable J.

A general class of squared distance functions is provided by utilizing positive definite quadratic forms. Specifically, if p represents a p-dimensional observation to be assigned to one of s groups, then to measure the squared distance between the observation  $\beta$  and the centroid (mean vector) of the i-th group one may consider the function

$$D_{i} = (\beta - \bar{x}_{i})^{T} M (\beta - \bar{x}_{i})$$

where M is a positive definite matrix to ensure that  $D_i \leq 0$ . Different distance functions are represented by different choices of the matrix M. When M = I (the identify matrix) the resulting metric is the standard Euclidean distance. Distances with the Euclidean metric are shown in Figure 1a. The variance within the data may make the unweighted Euclidean metric inappropriate. As shown on the Figure 1b, where X has a larger variance than Y,

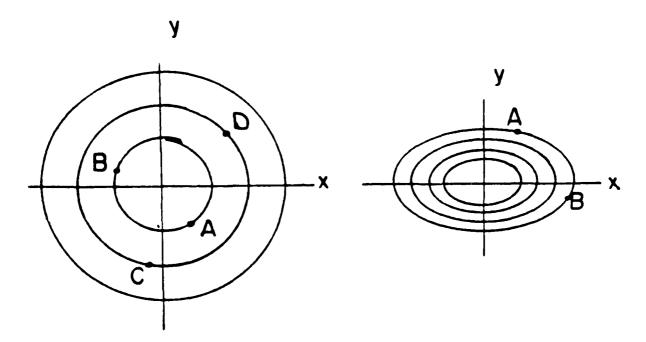
one may wish to weight a deviation in the X direction less than an equal deviation in the Y direction. This is a weighted Euclidean distance frunction which makes point A and B equidistance from the origin. In this case, the matrix M is diagonal elements which are the reciprocals of the variances of the different variables.

Extending this idea further, it may be possible to consider the covariance among variables as well. Figure 1c shows how the axis may be rotated so that the major axis is oriented in a direction of reflecting the positive correlation between X and Y. Again, points on the same ellipse are considered equidistance from the origin. The matrix M in this case is the inverse of the covariance matrix.

Further extension of this concept will expalin some sort of generalized distance function. If  $C_{\dot{1}}$  represents the covariance matrix of the  $\dot{1}$  th cluster then the distance function

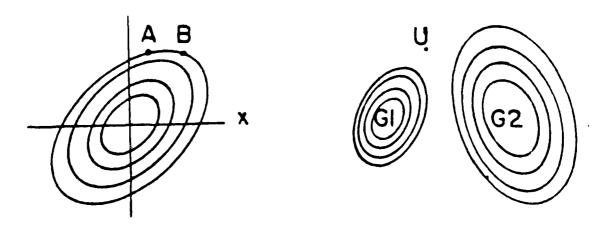
$$D_{i} = (\beta - \bar{x}_{i})^{T} C_{i}^{-1} (\beta - \bar{x}_{i})$$

uses the appropriate covariance structure when determining the distance to a particular cluster centroid. Since  $C_i$  changes to reflect the dispersion internal to each particular cluster, the use of this metric exploits differences in the dispersion characteristics of the different groups. As shown on Figure 1d, not how a new observation (denoted by u) is



la. Euclidean measure of squared distance.

lb. Measure of squared distance with different weights for variables.



lc. Generalized squared distance measure.

ld. Classification when withingroup dispersions are different.

Figure 1. Euclidean Distance

closer to the centroid of group one (G1) in terms of Euclidean distance but is more likely to be assigned to group two (G2) when using the  $C_{\hat{1}}$  matrix.

## 3. Mahalanobis Distance

Another choice for the M matrix in equation (1) is  $p^{-1}$  where P represents the pooled within groups covariance matrix of all the clusters.

$$P = \frac{1}{G (n_i - 1)} W$$

$$i = 1$$
(34)

where

$$W = \sum_{k=1}^{G} W_{k}$$

This distance is the well known Mahalanobis distance. Note that P does not change from group to group. To ensure the non-singularity of P it must be true that  $p \leq (N - G)$ , where N represents the total number of observations over all groups. Rewriting the distance,

$$D_{i} = (\beta - \bar{x}_{i})^{T} W^{-1}(\beta - \bar{x}_{i})$$
 (35)

defines a distance between mean vectors  $\beta$  and  $\bar{x}_i$  and common covariance matrix W. The Mahalanobis distance function adjusts for both scale of measurement of the variables and covariation among the variables. Use of this

metric is equivalent to computing distances on variables transformed to their principal components. This metric is invariant under any nonsingular transformation of original variables. For consider the transformation

$$Y = BX \tag{36}$$

and let  $D(Y_i, Y_j)$  represent Mahalanobis distance between  $Y_i$  and  $Y_j$  .

$$D(Y_{i},Y_{j}) = (Y_{i} - Y_{j})^{T} P_{Y}^{-1} (Y_{i} - Y_{j})$$

$$= (BX_{i} - BX_{j})^{T} P_{Y}^{-1} (BX_{i} - BX_{j})$$

$$= (X_{i} - X_{j})^{T} B^{T} P_{Y}^{-1} B(X_{i} - X_{j})$$

$$= (X_{i} - X_{j})^{T} B^{T} (BP_{X}B^{T})^{-1} B(X_{i} X_{j})$$

$$= (X_{i} - X_{j})^{T} P_{X}^{-1} (X_{i} - X_{j})$$

$$= D(X_{i}, X_{j})$$

Some other common metrics are listed below:

- 1.  $L_1$  norm (City Block)  $D(X_i, X_j) = \sum_{k=1}^{p} |X_{ki} X_{kj}|$
- 2.  $L_p$  norm (Minkowsky Metrics)  $D(X_i, X_j) = (\sum_{k=1}^{p} |X_{ki} X_{kj}|^p)^{1/p}$

### 3. Uniform norm

$$D(X_i,X_j) = \underset{k=1,2,\ldots,p}{\text{Superemum}} \{|X_{ki} - X_{kj}|\}$$

### C. HIERARCHICAL CLUSTERING

### 1. General

The previously discussed distance measures may be used to construct a similarity matrix describing the length of all pairwise relationships among the entities (variables or data units) in the data set. The methods of hierachical cluster analysis operate on this similarity matrix to construct a tree depicting specified relationships among the entities. As shown on Figure 2, the branches on the left each represent one entity while the root represents the entire collection of entities. Moving down the tree from the branches toward the root depicts increasing aggregation of the entities into clusters. Hierarchical clustering methods which build a tree from branches to root often are called agglomerative methods.

Once a tree is constructed for N entities, the analyst may choose from as many as N sets of clusters. These clusters are nested. From the agglomerative view, when two entities are merged they are joined together permanently and considered as one entity for later merges; from the divisive view, when a group of entities is split into two parts, the parts are separated permenently and may be treated independently for the remainder of the analysis.

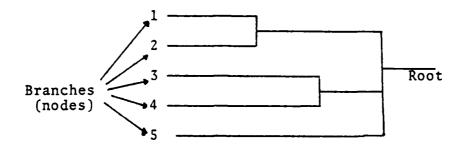


Figure 2. Tree for Hierarchical Clustering

Herein lie both the strength and weakness of hierarchical methods: by taking early decisions as permanent, the number of posibilities that need be examined is reduced greatly as compared with complete enumeration; but this same convention precludes discovering early mistakes or capitalizing on later opportunities.

There are three major hierarchical clustering concepts:

- 1. Linkage Methods
- 2. Centroid Methods
- 3. Error sum of squares or variance methods.

All of these methods are suitable for clustering data units. However, only the linkage methods are considered in this research.

# 2. The General Agglomerative Procedure

Let  $s_{ij}$  be the similarity between entities i and j as defined by one of the distance measures previously discussed. Assuming that the similarity is symmetric, the complete schedule of similarities for all  $\binom{N}{2} = \frac{1}{2}N(N-1)$ 

possible pairwise combinations of entities may be arrayed in a lower triangular similarity matrix as in Figure 3. The  $s_{ij}$  entries are nonnegative. This limitation is of consequence only for correlation and the cosine of the angle between vectors; the distinction between positive and negative association cannot be utilized in these clustering methods.

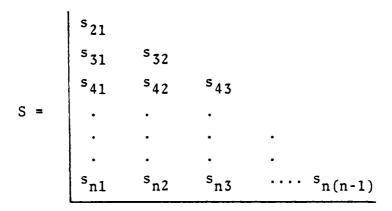


Figure 3. Lower Triangular Similarity Matrix

A simple remedy is to use the absolute value or the square of the measure if it can assume negative values. Once the matrix is defined, the process of clustering entities is almost trivially simple. The general procedure for agglomerative clustering on a data matrix is as follows:

(1) Begin with n clusters each consisting of exactly one entity. Let the clusters are labled with the numbers 1 through N.

- (2) Search the similarity matrix for the most similar pair of clusters. Let the chosen clusters be labeled p and q and let their associated similarity be  $s_{pq}$ , p > q.
- (3) Reduce the number of clusters by 1 thorugh merger of clusters p and q. Label the product of the merger q and update the similarity matrix entities in order to reflect the revised similarities between cluster q and all other existing clusters. Delete the row and column of S pertaining to cluster p.
- (4) Perform steps 2 and 3 a total of N-1 times

  (at which point all entities will be one
  cluster). At each step record the identity
  of the clusters which are merged and the value
  of similarity between them in order to have
  a complete record of the results.

Different agglomerative methods are implemented by varying the procedures used for defining the most similar pair at step 2 and for updating the revised similarity matrix at step 3. The similarity matrix is a given array of numbers. The numerical execution of the clustering procedures is completely independent of how the similarity values were generated or whether the entities to be clustered are variables or data units. However, it is necessary to make a direct distinction between distance-like

measures (the smallest values correspond to the most similar pairs) and correlation-like measures (the largest values correspond to the most similar pairs); the essential difference is whether the search for the most similar pair involves seeking the minimum or maximum entry in the similarity matrix.

# 3. Single Linkage

The method of single-linkage cluster analysis is the simplest of all hierarchical techniques. At each stage, after clusters p and q have been merged, the similarity between the cluster (labeled t) and some other r is determined as follows:

1. If s<sub>ii</sub> is the distance-line measure

$$s_{tr} = \min (s_{pr}, s_{qr})$$
 (37)

The quantity  $s_{tr}$  is the distance between the two closest members of clusters t and r. If clusters t and r were to be merged, then for any entity in the resulting cluster the distance to its nearest neighbor would be at most  $s_{tr}$ .

2. If  $s_{ij}$  is a correlation-like measure

$$s_{tr} = \max (s_{pr}, s_{qr})$$
 (38)

The quantity  $s_{tr}$  is the similarity between the two most similar entities in clusters t and r. If clusters t

and r were to be merged, then for any entity in the resulting cluster there would be at least one other entity in the same cluster such that the pair would have a similarity at least as large as  $s_{+r}$ .

The method is known as single linkage because clusters are joined at each stage by the single shortest or strongest link between them. Since the updating process involves choosing only the minimum or maximum single-linkage clustering is invariant to any transformation which leaves the ordering of the similarities unchanged; that is, any monotonic transformation.

# 4. Complete Linkage

The complete-linkage method is related to the single-linkage method and is no more difficult to execute. At each stage, after clusters p and q have been merged, the similarity between the new cluster (labeled t) and some other cluster r is determined as follows:

1. If s<sub>ii</sub> is distance-like measure

$$s_{tr} = \max (s_{pr}, s_{qr})$$
 (39)

The quantity  $s_{tr}$  is the distance between the most distant members of clusters t and r. If clusters t and r were merged, then every entity in the resulting cluster would be no farther than  $s_{tr}$  from every other entity in the cluster. The value of  $s_{tr}$  is the diameter of the samllest sphere which can enclose the cluster resulting from the merger of clusters t and r.

2. If  $\boldsymbol{s}_{\underline{i}\cdot j}$  is a correlation-like measure

$$s_{tr} = \min (s_{pr}, s_{qr})$$
 (40)

The quantify  $s_{tr}$  is the similarity between the two most dissimilar entities in clusters t and r. If clusters t and r were to be merged, then every entity in the resulting cluster would have a similarity of at least  $s_{tr}$  with every other entity in the cluster.

The method is called complete linkage because all entities in a cluster are linked to each other at some maximum distance or minimum similarity. Such a cluster is called a "maximally connected subgraph" in graph theory. In contrast to the single-linkage method, interpretation of the clusters can be made only in terms of the relationships within individual clusters; there is no particularly useful interpretation involving the differences between clusters. Like the single-linkage method, complete-linkage cluster analysis is invariant to monotonic transformations of the similarity measure. Johnson (1967) discusses this property in both single and complete linkage methods.

### D. NONHIERARCHICAL CLUSTERING

Nonhierarchical clustering methods are designed to cluster data units into a single classification of g clusters, where g either is specified a priori or is determined as a part of the clustering method. The central idea in most of these methods is to choose some initial

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partition of the data units and then alter cluster memberships so as to obtain a better partition. The various algorighms which have been proposed differ as to what constitutes a "better partition" and what methods may be used for achieving improvements.

The broad concept for these methods is very similar to that underlying the steepest descent algorithms used for unconstrained optimization in nonlinear programming. Such algorithms begin with an initial point and then converge to a local optimum, moving one step at a time, the value of the objective function improving at each step.

The methods of nonhierarchical clustering typically may be used with much larger problems than the hierarchical methods because it is not necessary to calculate and store the similarity matrix; it is not even necessary to store the data set. In general, the data units are processed serially and can be read from tape or disk as needed. This characteristic makes it possible, at least in principle, to cluster arbitrary large collections of data units.

In this research, we consider only the partitioning method known as "K-MEANS" which was developed by MacQueen (15). He used the term "K-MEANS" to denote the process of assigning each data unit to that cluster (of k clusters) with the nearest centroid (mean vector). The cluster centroid changes with each transfer of an observation.

The decomposition of the total scatter matrix into within and between groups matrices suggests possible

optimality criteria to be used in a clustering algorithm.

One would like the within-groups scatter to be small relative to the between-groups scatter. Various trial clusterings could be formed using the W and B matrices as a basis for the optimality criteria which determine the best clustering. A possible choice for a criterion is to minimize trace W over all partitions into g groups.

Since T is constant over all partitions, minimizing trace W is equivalent to maximizing traces B since

trace 
$$T = trace W + trace B$$
 (41)

Although trace W is invariant under an orthogonal transformation, it is not invariant under other non-singular linear transformations.

McRae (16) points out that trace  $\,W\,$  equals the total within group sum of squares, hence the "minimum variance partition" cluster solution is found by minimizing trace  $\,W\,$ .

Considerable study has been developed to alternative criteria such as those based on multivariate statistical analysis techniques, especially the methods of linear discriminant analysis and multivariate analysis of variance. Assuming the  $\,p\,$  variables are not linearly dependent, then as long as  $\,p\,$  =  $\,N\,$  -  $\,g\,$  ,  $\,W\,$  is positive definite symmetric and so is  $\,W^{-1}\,$ . Attempts to make  $\,B\,$  and  $\,W\,$  as different as possible lead one to solving the determinantal equation:

$$|B - \lambda W| = 0 \tag{42}$$

The solutions  $\lambda_i$  are the eigenvalues of the matrix  $W^{-1}B$ as in discriminant analysis. There are t non-zero eigenvalues, where t is the minimum of p and g-1. This is a consequence of the fact that, if g is less than p, the g group means are considered in a (g-1)-dimensional hyperplane. When g = 2 the analysis is equivalent to two-group discriminant analysis. Linear discriminant analysis would take the vectors originally described in p-dimensional coordinate system and transform the basis to a t-dimensional system. Maximizing the largest of these eigenvalues is a criterion suggested by S.N. Roy and maximizing the trace of W<sup>-1</sup>B, however is a criterion suggested by Hotelling. In both cases, large values for these statistics are sought in clustering algorithms since large values indicate large differences among (between) groups. Minimizing the ratio of determinants  $|W| \div |T|$ is a criterion widely known as Wilks' lambda discussed in the discriminant analysis. Since T is the same for all partitions, this criterion is equivalent to minimizing determinant W. Both trace  $W^{-1}B$  and  $|T| \div |W|$ be expressed in terms of the eignevalues of  $W^{-1}B$ .

$$\begin{vmatrix} T \\ \overline{W} \end{vmatrix} = \frac{t}{\pi} (1 + \lambda_i)$$

$$i = 1$$
(43)

trace 
$$W^{-1}B = \sum_{i=1}^{t} \lambda_i$$
 (44)

where t = min(p, g-1) . Therefore minimizing det W is equivalent to maximizing  $\pi(1 + \lambda_i)$ .

Friedman and Rubin (6) describe the advantages of the various criteria. Those based on multivariate statistical considerations (all but trace W) are invariant under changes in scale for varibles (non-singular linear transformation). In fact, they are the only invariants for W and B under such transformations. In addition, the multivariate criteria may take into account covariation among the variables.

## V. ANALYSIS OF MULTIVARIATE UTILITY DATA

To illustrate hierarchical clustering we applied the technique described in the previous chapter to partition a set of twenty six attributes of a close-air support weapon system into a smaller collection of "superattributes". As part of an effort to evaluate the military utility of a proposed alternative U.S. Marine Corps air support rada system, AN-TPQ/27. Barr and Richards (4) extracted 26 attributes of the TPQ-27 and a baseline system, the AN-TPQ/10, and then had members of the Operational Test and Evaluation Team assess the utility of the TPQ/27 relative to that of the TPQ/10. In order that the additive model used to combine unidimensional relative utilities into a system relative utility be justifiable, it is necessary that the utilities satisfy certain independence properties described in Keeney and Raiffa (12).

Because those independence properties are very difficult for decision makers to verify for complex alternatives like the weapon systems under study, Professors Barr and Richards attempted instead to work with the attributes to try to generate a new collection which would likely satisfy, at least approximately, the conditions required to justify the additive model.

The original collection of 26 attributes is as follows:

- 1. Portability
- 2. Durability
- 3. Time to Set Up
- 4. Time to Take Down
- 5. Ease of Assigning Aircraft to Targets
- 6. Number of Aircraft Controlled
- 7. Number of Targets
- 8. Communications
- 9. Mission Flexibility
- 10. ASRT Survivability
- 11. Time to Locate and Acquire Aircraft
- 12. Accuracy of Tracking
- 13. Accuracy of Delivery
- 14. Range
- 15. Aircraft Vulnerability
- 16. Aircraft Attack Throughout
- 17. Base of Adjustment and Evaluation of Results
- 18. Accuracy of Feedback
- 19. Ease of Operation
- 20. Man-Machine Compatibility
- 21. Training Requirements
- 22. Reliability
- 23. Maintainability
- 24. Supportability
- 25. Availability
- 26. Documentation

where a; represents an attribute i and

$$I(x_{ij}, x_{kj}) = \begin{cases} 1 & \text{if } x_{ij} = x_{kj} \\ 0 & \text{if } x_{ij} \neq x_{kj} \end{cases}$$

It is easy to verify that D is a metric as defined in Chapter IV. Since we will actually work with a similarity measure in the hierarchical cluster procedure, we define the similarity between two attributes  $a_i$  and  $a_k$  as

$$S(a_i, a_k) = \sum_{j=1}^{12} I(x_{ij}, x_{kj})$$
 (46)

One can see from this definition that the similarity between two attributes  $a_i$  and  $a_k$  is simply the number of team members who placed attributes  $a_i$  and  $a_k$  in the same partition. For example,

Either S or D can be used in the computer program shown in Appendix A for hierarchical clustering. One need only indicate whether he wants a correlation-like (larger values imply more similar) measure or a distance-like measure (smaller values imply more similar). We selected to use the former method. The similarity matrix extracted from

Table II. Data Matrix

										•			
_	1	2	3	4	5	6	7	8	9	10	11	12	_
1	6	2	1	3	2	4	3	1	3	1	1	1	
2	1	2	2	3	1	3	2	1	1	5	1	2	
3	6	1	1	5	2	4	3	1	6	1	2	1	
4	6	1	1	5	2	5	3	1	6	1	2	1	
5	2	5	3	1	3	1	1	2	2	2	3	3	
6	2	7	4	1	4	1	1	2	4	2	3	3	
7	2	7	4	1	4	1	1	2	4	2	3	3	
8	3	5	4	7	5	6	1	3	1	3	3	6	
9	2	5	4	1	3	1	1	2	4	2	3	3	
10	9	6	5	6	5	7	8	3	7	3	2	4	
11	2	8	6	4	3	2	1	4	4	2	3	3	
12	3	8	7	4	4	2	6	5	4	6	4	3	
13	3	8	7	4	4	2	6	5	4	6	4	3	
14	3	8	4	4	4	2	6	5	4	2	4	3	
1\$	7	6	5	6	5	7	7	3	7	3	7	4	
16	8	8	6	1	4	1	7	4	4	2	7	3	
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21	5	4	9	2	3	8	4	7	2	4	6	5	
22	1	3	2	3	1	3	2	7	1	5	6	2	
23	1	3	9	3	1	3	2	7	1	5	6	2	
24	1	3	4	3	1	3	2	7	3	5	6	2	
25	1	3	2	3	1	3	2	7	1	S	6	2	
26	5	4	9	2	6	8	4	7	2	4	6	5	

from the data is shown in Table V-3. We present only lower triangular elements since  $S(a_i, a_i) = 12$  for all i and the matrix is symmetric; i.e.,  $S(a_i, a_k) = S(a_k, a_i)$ . Zero values are not written.

The results from the hierarchical clustering are shown in Figure 4. The numbers printed along the left hand margin refer to the attribute numbers. As you proceed to the right through the tree you will observe numbers greater than 26. These correspond to the clusterings that takes place from one step to the next. For example, the number 27 shown at the juncture of 25 and 22 means that the first attribute clustered together should be 25 and 22 (this is the most similar pair). This combination is then considered as a new attribute which is later combined with the attribute 30 (itself a combination of 23 and 24) to form the attribute 31. This is later combined with attribute 2 to form attribute 40, etc.

As discussed in Chapter IV a decision has to be made as to how many clusters (superattributes) are desired. All hierarchical methods will continue clustering until there is a single cluster. In order to decide on the number of clusters (and their composition) one need only image drawing a vertical line through the tree at various places. Each intersection of the tree with the vertical line results in a cluster. For example, teh vertical line at the point A results in the 6 clusters shown in Table V-4.

It is clear from observing the above collection that some of the attributes are highly correlated and nonredundant. If one tries to assign an importance weights to each attributes separately, there is a distinct likelihood that some of the overlapping strongly into related attributes might effectively be double or triple weighted or more producing biased result. It is an effort to prevent this from happening, Barr and Richards aksed the utility assessment team to partition the 26 attributes into a smaller collection in such a way that attributes within a group are similiar and attributes in different groups are unrelated the sense that utility assessments for attributes in one group do not depend on the amounts of attributes in any other group.

The total number of groups was not prespecified. Instead, each team member was allowed to partition the 26 attributes into any number of groups. The resulting multivariate data array is shown in Table V-2. An element  $\mathbf{x}_{ij}$  is the number of the group into each team member j put attribute i.

Let us define a distance measure for this data array as follows:

$$D(a_{i}, a_{k}) = \sum_{j=1}^{12} (1 - I(x_{ij}, x_{kj}))$$
 (45)

Table III. Similarity Matrix for Superattribute Determination.

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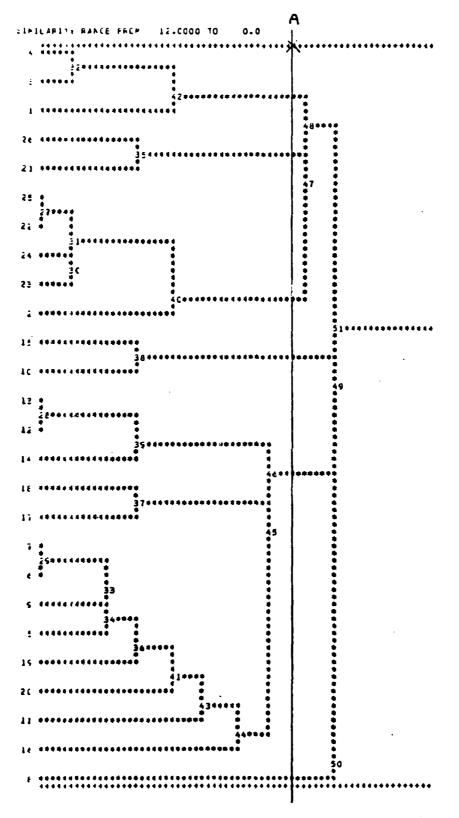


Figure 4. Tree for 26 Attributes

The superattributes used in the utility study are those sohwn in Table IV. A careful examination of the attributes which comapre the clusters shows that the results so obtained are intuitively agreeable. The names supplied to the superattributes are somewhat natural descriptions of the clusters obtained.

The listing of the computer program and sample output are given in Appendix A.

# Table IV. Superattributes

Superattributes	Component Attributes
Facility of movement	<ol> <li>Portability</li> <li>Time to set up</li> <li>Time to take down</li> </ol>
Facility of Use	5. Ease of assigning
(precision)	aircraft to targets 6. Number of aircraft controlled 7. Number of targets 9. Mission flexibility 11. Time to locate and acquire aircraft 16. Aircraft attack
	throughput 17. Ease of adjustment 18. Accuracy of feedback 19. Ease of operation 20. Man-machine compatibility 12. Accuracy of tracking 13. Accuracy of delivery 14. Range
Survivability	10. ASRT Survivability 15. Aircraft vulnerability
Learning	21. Training requirements 26. Documentation
Readiness	2. Durability 22. Reliability 23. Maintainability 24. Supportability 25. Availability
Communications	8. Communications

# VI. ANALYSIS OF ARMY TANK DATA

### A. DATA STRUCTURE

In order to illustrate the nonhierarchical clustering methodology, principal components analysis, and discriminant analysis data on Army tanks from eight different countries were taken from Jane's Book of Weapon Systems (1979-80). A total of twenty-four tanks were included in the data array with observation on each of 10 variables. The 10 variables are listed below:

- 1. Weight (ton)
- 2. Length (meter)
- 3. Width (meter)
- 4. Height (meter)
- 5. Road Speed (kilometer per hour)
- 6. Trench Crossing (meter)
- 7. Ground Pressure (Kg/cm<sup>2</sup>)
- 8. Maximum Armament (rounds)
- 9. Ground Clearance (meter)
- 10. Power to Engine Ratio (BHP/ton)

The twenty-four tanks and the associated countries are shown below:

Identification Number	Type/Name	Country
11	T-62	
12	T-54	U.S.S.R.

Identification Number	Type/Name	Country
13	T-10	· · · · · ·
14	ASU-85	
15	MK-5/Chieftain	
16	MK-3/Vickers	
17	MK-13/Centurion	U.K.
18	CVR(T)/Scorpion	
19	XM-1	
20	M60A2	
21	M60	U.S.A.
22	M4 8	
23	M4 7	
24	PZ61	CWITZED
25	PZ68	SWITZER- LAND
26	STRV-103	SWEDEN
27	Ikv-91	SWEDEN
28	TYPE61	TADAN
29	TYPE74	JAPAN
30	Leopard 2	
31	Leopard	W. GER-
32	TAM	MANY
33	AMX 30	EDENCU
34	AMX 13	FRENCH
	<del></del>	

We conjecture that a cluster analysis of the tank data will result in clusters corresponding to nationality since the nations may have different emphasis on the variables in the design of their tanks.

### B. NONHIERARCHICAL CLUSTER ANALYSIS OF TANK DATA

## 1. The MIKCA Algorithm

The specific algorithm chosen for the nonhierarchical cluster analysis for the tank data is the MIKCA (Multivariate Iterative K-MEANS Clustering Algorithm) program written by Douglas J. McRae as a part of his doctoral dissertation at the University of North Carolina, Chapel Hill.

Reference to the flow chart in Figure 5 will aid the reader in following discussion of the algorithm. Inputs to program are the data matrix, an estimate for g (the number of clusters), and choice of criterion and distance functions.

In the first step, preliminary claculations are made, such as the variable means and standard deviations, as well as the cross product matrix T. The next step forms the initial cluster centers. Then each of the other observations is assigned to the nearest cluster. Euclidean distance is used for this initial phase, and the cluster centroids are recomputed after each observation is assigned to a group. The observations are considered in the same order as they were input. After all of them have been assigned to clusters, the criterion value is computed. This initial cluster-finding technique is referred to as a

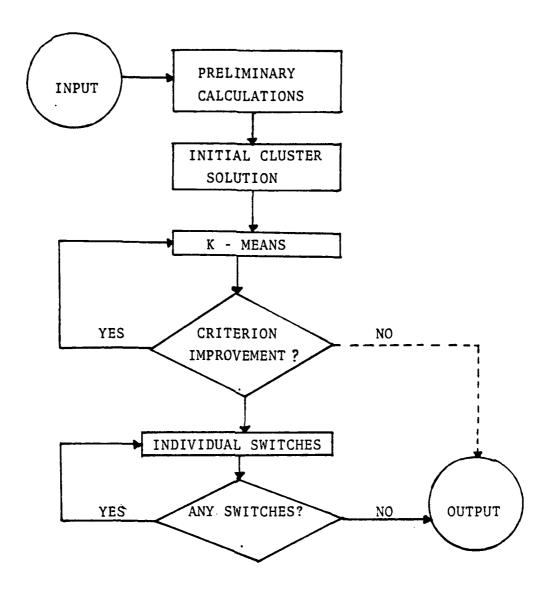


Figure 5. MIKCA Flow Chart

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one-pass K-MEANS procedure. It is performed three times, and the solution which yields the best criterion value is chosen as the initial cluster solution.

After the initial solution has been found, the program advances to the iterative K-MEANS phase where the observations are again considered in the order in which they were input to the program. It is this phase where the user's choice of distance function is used. The distance from each observation to each cluster centroid is again computed, this time with the user's distance function, the assignment to the closest centroid being made and the centroid updated to reflect its new membership. After considering all n observations in this manner, the new criterion value is checked for possible improvement during the K-MEANS iteration. As long as the criterion value improves, the K-MEANS procedure is repeated; if the criterion fails to improve then the MIKCA algorithm goes to the next step, the individual switches section. Note the importance of the order of consideration of the observations. The order is important because the cluster means are recomputed after each observation is reassigned.

In the individual switches phase, consideration is given to moving each observation to every other cluster, the move being made if and only if an improvement in the value of the criterion results. An elaborate labelling procedure provides a unique order in which to consider each observation. This procedure continues until a complete pass through the data is made with no changes in cluster membership.

The MIKCA alogorithm provides the following options for distance and criterion functions.

### Criterion

- 1. Minimum trace W
- 2. Minimum determinant W
- 3. Maximum largest order of  $|B \lambda W| = 0$
- 4. Maximum sum of roots of  $|B \lambda W| = 0$

#### Distance

- 1. Euclidean
- 2. Weighted Euclidean
- 3. Mahalanobis

A complete computer program is listed in Appendix B.

## 2. Cluster Results for Tank Data

For clustering of the tank data we selected the minimum trace W criterion and the weighted Euclidean distance function. The algorithm automatically provides weights for the weighted Euclidean distance function.

The results of the clustering with four clusters are shown in Table V.

The conjecture of clustering by nationalities is supported by the results. The three Soviet tanks make up one cluster and the two British and four of the United States tanks were found to be similar. A third cluster consists of four tanks which are very lightweight. The

Table V. THE FINAL CLUSTER SCLUTION IS

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final cluster consists of the rest of the tanks, including tanks of United States allies from West Germany, France, Sweden, Switzerland and Japan.

A natural question to ask after observing the results of a cluster analysis is what variables most strongly influence the clustering that was observed. A clue is provided by the composition of the cluster containing all of the lightweight tanks. This suggests that weight is an important distinguishing feature. This is examined in the principal components analysis and the discriminant analysis in the next two section.

## C. PRINCIPAL COMPONENTS ANALYSIS

The Statistical Package for Social Sciences (SPSS)

(14) subprogram FACTOR was used for the principal components analysis. It is designed both for the factor analysis and the principal components analysis. The outputs are designed to be self-explanatory. In this example, the first 5 components accoung for 90% of the variance and the remaining components account for only 10% of the variance (Figure 6).

The subprogram FACTOR provides a graphical presentation (Figure 7) for the factors that have been determined by the orthogonal rotations (in this example, variance maximization rotation). In reading the graphs, one should be attentive to following three features: (1) the relative distance of a variable from the axis, (2) the direction of a variable in relation to the axis, and finally (3) clustering of variables and their relative position to each other.

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Summary Table of Principal Components Analysis on Tank Figure 6.

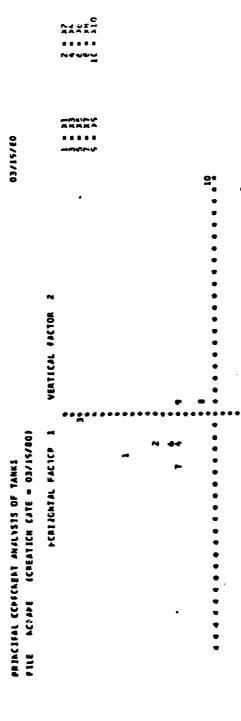


Figure 7. Graphical Presentation

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Figure 8. Factor Score Coefficients

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For example, variables 5 (road speed) and 10 (power to engine ratio) contribute heavily to the first principal component while variables 1 (wieght) and 3 (width) contributes most strongly to the second principal component. Variables 2, 4, 6, 7, 8, 9 are not as important. The weights accorded each variable in the 10 factors (principal components) are shown in Figure 8. The complete SPSS program is listed in Appendix C.

## D. DISCRIMINANT ANALYSIS

The SPSS subprogram DISCRIMINANT was used to determine that function or those functions of the 10 variables that best discriminant among the four clusters determined in previous section.

The maximum number of discriminant functions to be derived is either one less than the number of groups or equal to the number of discriminating variables. This subprogram provides two measures for judging the importance of discriminant functions. One of these is the relative percentage of the eigenvalue associated with the function. It is a measure of the relative importance of the function. The sum of the eigenvalues is a measure of total variance existing in the discriminating variables. Since discriminant functions are derived in order of their importance, this process can be stopped whenever the relative percentage is judged to be too small. Of course, there is no fixed rule for deciding whatis too small. In this research, we selected arbitrary, a significance level of 0.10. The output shown

in Figure 9 suggests that we therefore consider only the first two discriminant functions.

The second measure judging the importance of a discriminant function is its associated canonical correlation. The canonical correlation is a measure of association between the single discriminant function and the set of (g-1) dummy variables which define the g group memberships. It tells us how closely the function and the group variable are related, which is just another measure of the function's ability to discriminate among the groups. From Figure 10, the first two discriminant functions are each highly correlated with the groups but the third has only a moderate correlation.

The next criterion for eliminating discriminant functions is to test for the statistical significance of discriminating information not already accounted for by the earlier functions. As each function is derived, starting with no (zero) functions, Wilks' lambda is computed. Lambda is an inverse measure of the discriminating power in original variables which has not yet been removed by the discriminant functions - the larger lambda is, the less is the information remaining. Lambda can be transformed into a chi-square statistic for an easy test of statistical significance. In Figure 9, Wilks' lambda was .594 after the first two functions had been derived. This corresponds to a chi-square of 8.8476 with a probability level of .1823.

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Figure 9. Summary Table of Discriminant Analysis on Tank

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Canonical Discriminant Function Coefficients Figure 10.

This means that a lambda of this magnitude or smaller has a .1823 probability of occurring due to the chances of sampling even if there was no further information to be accounted for by a third function in the population.

Clearly, a third function is not statistically significant in this case.

The standarized discriminant function coefficients corresponding to the values of the  $v_{ij}$ 's discussed in the previous section are used to compute the discriminant score for a case (observation) in which the original discriminating variables are in standard form. The discriminant score is computed by multiplying each discriminating variable by its corresponding coefficient and adding together these products. There is a separate score for each observation on each function. The coefficients have been derived in such a way that the discriminant scores produced are in standard form.

When the sign if ignored, each standard discriminant function coefficient represents the relative contribution of its associated variable to that function. The sign merely denotes whether the variable is making a positive or negative contribution.

A graphical presentation is shown in Figure 11 using the first and the second canonical discriminant function as the axis. From this scatterplot, we can easily see that Soviet tanks (labelled 1) are well distinguished from the all of the others using only the first two discriminant

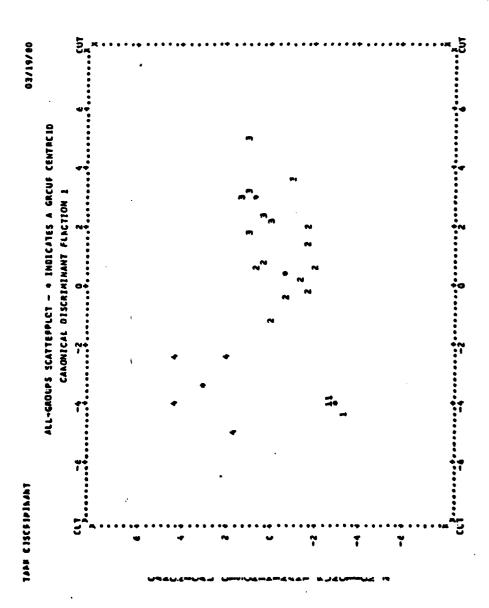


Figure 11. Scatter Plot for all Groups

functions. Also, all the lightweight tanks are clearly separated from the others. The distinction between groups 2 and 3 is also clear though not separated from each other as much as from groups 1 and 4. The complete SPSS program for the discriminant analysis is listed in Appendix D.

## VII. CONCLUSION

The multivariate analysis techniques of cluster analysis, principal components analysis and discriminant analysis are useful in real world problems for examining observations on each of several dimension. Each of the techniques is related mathematically to the others, and each complements the other in explaining the data.

Computer software is readily available in many sources. The software used in this thesis for hierarchical clustering, principal components analysis, and discriminant analysis was from the IMSL package and SPSS. For nonhierarchical clustering, we used the FORTRAN program developed by McRae (16). All of this software is readily available and documented at the Naval Postgraduate School.

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7. REVERSALS (IER=130) MAY CCCLR IN THE WAYS. FIRST, THE NCDES MAY BE JCINED AT A LOWER LEVEL (CLOSER TO YSIM(1)). SECOND, THE LEVEL OF THE HEAD ADDE MAY LIE ABOVE THE INTERVAL (YSIM(2)). YSIM(2)). WIN(2)). WIN(2)). THE TREE CREATED BY USTREE SHOULD BE TURNED TO AN UFRIGHT POSITION.
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GC hFITE(6,2) (CLEVEL(I), ICLSCA(I), ICFSOA(I), I=1,25)
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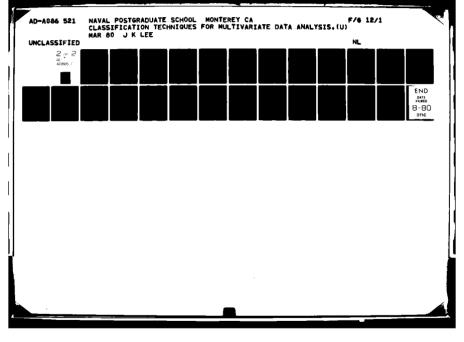
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<u>, , ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,</u>	PEFCRE TEE SELTCH EAS CCASIDERED  A ISVT(ANEW) = NISV(ANEW)  A ISVT(ADLD) = NISV(ACLO)  C 665 J=1,*VARS  S C C C C C C C C C C C C C C C C C C	FINISH WITH CLUSTER M: IF NG SWITCHES HAVE EEEN MADE, SET JELAG(M) = 2 AND GC TC NEXT CLUSTER; IF SWITCHES HAVE BEEN MACE ADJUST LSTSV AND SET JELAG(M) = C AND GO TC NEXT CLUSTER 655 JFLAG(M) = C C O GO TO 699 = C AND GO TO NEXT CLUSTER 655 JFLAG(M) = C C O GO TO 699 = C AND GO TO NEXT CLUSTER	DONE HITH ALL CLUSTERS: IFLAG = 1 MEANS SCME SWITCHES HAVE BEE MALE: GO BACK AND ITERATE If (IFLAG.EG.1) GC TO 6CO All DONE: ACCURATELY CALCULATE MEANS AND CRITERICA AND CLIFUI	75C HRITE (6,90C) SCC FCRMAT (11,1,1HE FINAL CLUSTER SCLUTION IS 1)	NECALCULATE CLOSTER CENTERS, WITTIN-CLOSTERS FAIRTY, AND CRITCHIS VC 715 J=1,NGPS 715 S(CEN(M,J) = 0. 715 S(CEN(M,J) = 0. 0 720 1=1,008S	CC 720 JELINVARS 2C SICEN(M,J) = SVCEN(W,J) + DATA(I) JINISV(M CALL WCALC (SVCEN,NISV,NGPS,IDIR) IF (IFINE EC.I) RETURN CALL CRITON (CRIT)	IF (IFINE EC.I) RETURN CALL THE OUTFUT ROLTINE CALL GOOD (CRIT) WRITE (6,501) SCI FCRMAT ('0 END OF CLUSTER PROBLEP* RETURN	ENC SLBROUTINE CUTPUT (CRIT) THIS SUBRCLIINE PRINTS OUT THE CLUSTER SIZE FOR EACH CLUSTER — THE CLUSTER SIZE

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2CC CFT = 1. CC 205 J=1.NVARS 2C5 CET = DET*WFCT(J,J) CFIT = CET RETURN	CALCULATE LARGEST ROOT AS L(INV)*E*L*(INV) WHERE L IS THE CHCLESKY FACTOR OF W CHCLESKY FACTOR OF W CAITERICN IS RECIFROCAL OF LARGEST ROOT	300 CC 305 J=1,NVARS CC 305 K=J,NVARS BT(J,K) = B(J,K) BT(J,K) = BT(J,K) CALL (TISUI (NVARS, ET, WFCT) CALL ETGN (NVARS, ET, ETG, VEC, IND) RETURN	CALCULATE PCTELLING'S TRACE AS SUM OF DIAGONAL ELEMENTS CF LINV)*8*L'(INV) CFITERION IS RECIFRCCAL OF THIS SUM	4CC CC 405 J=1. NVARS CC 405 K=J+NVARS DI 405 K=J+NVARS	4C5 E1(K,J) = B1(J,K) CALL UTISUI (NVARS,BT,WFCI)	41C CFIT = CRIT+8T(J,J) CFIT=1.0/ CFIT FETURN	(SV, NI,NGP, IDIR)	THIS SUBRCUINE CALCULATES THE WITHIN-CELLS WATRIX AND, IF NECESSARY, THE CHULESKY FACTOR OF THE WITHIN-CELLS MATRIX	CCMMCN NOPS, NVARS, NGPS, ICRIT, NOSTAN, IDIST, IFINE, KTIPE, ICENT(6CC), 1CATA(6CC), 201, T(2O, 2O), B(2O, 2O), M(2O) 201, WFCT(2O, 2C), SVCEN(2O), 201, TSV(2C), NWEAN(2C), SC(2O), NVEC(2C), TVEC(2C), SVCENT(2O, 2O), NMEAN(2C), SC(2C), NVEC(2C), TVEC(2C), TVEC(2C), BT(2C), 2O), CIPENSICN S\((2C), NI(2O), NI(	CALCULATE B AND THEN W = T - B B = SLW NISN(M) *SVCEN(M) **2
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IF (K . EC. 1) GO TC 190

CC 180 J=2,K

IF (AK) Z10,200,210

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I)-W1AW#h(1)
PAF_MATRIX, REQUIRED PART
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[I+1,J+1]=A(I+1,J+1)-2.*(W(I)*QJ+hJ*O(I))
ETA(NR)=B
ETASQ(NR)=E*B
FFMA(NF+1)=A(NR+1,NR+1)
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SCW=C 120 I=NR,NI SCW=C 180 J=NR,I (11,J+1)*W(J) I=I+1 I=I+1 I=I+1 11,J+1)*W(J) If (NI-II) 210.100
                                                                                                                                                           NI-II) 210,150,190
200 J=II,NI
=SUM+A(J+1,I+1)*W(J)
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